chain nodes : 16 17 18 19 20 21 22 23 24 25 26 39 40 41 ring nodes : 9 10 11 12 13 14 27 28 29 30 31 32 33 34 35 1 2 3 4 5 6 7 8 36 37 38 chain bonds : 2-22 3-20 4-21 6-26 7-16 9-24 10-17 11-25 12-19 12-23 13-18 17-28 18-27 29-40 30-39 31-44 35-42 35-45 36-41 37-46 39-43 ring bonds : 1-2 1-11 2-3 3-4 4-5 5-12 6-7 6-10 7-8 8-14 9-10 9-13 11-14 12-13 27-29 27-33 28-34 28-38 29-30 30-31 31-32 32-33 34-35 35-36 36-37 37-38 exact/norm bonds : 3-20 7-16 10-17 12-19 13-18 17-28 18-27 29-40 30-39 36-41 exact bonds : 1-2 1-11 2-3 2-22 3-4 4-5 4-21 5-12 6-7 6-10 6-26 7-8 8-14 9-10 9-13 9-24 11-14 11-25 12-13 12-23 27-29 27-33 28-34 28-38 29-30 30-31 31-32 31-44 32-33 34-35 35-36 35-42 35-45 36-37 37-38 37-46 39-43 isolated ring systems : containing 1 : 27 : 28 :

## Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS

Page 3

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STF

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 09:01:02 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1389 TO ITERATE

100.0% PROCESSED 1389 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L2 0 SEA SSS FUL L1

=>

Uploading C:\STNEXP4\QUERIES\10-648946a.str

chain nodes :

16 17 18 19 20 21 22 23 24 25 26 39 40 41 42 43 44 45 46 ring nodes :  $1 \ \bar{2} \ 3 \ 4 \ 5 \ 6 \ 7 \ 8 \ 9 \ 10 \ 11 \ 12 \ 13 \ 14 \ 27 \ 28 \ 29 \ 30 \ 31 \ 32 \ 33 \ 34 \ 35$ 36 37 38 chain bonds : 2-22 3-20 4-21 6-26 7-16 9-24 10-17 11-25 12-19 12-23 13-18 17-28 18-27 29-40 30-39 31-44 35-42 35-45 36-41 37-46 39-43 ring bonds : 1-2 1-11 2-3 3-4 4-5 5-12 6-7 6-10 7-8 8-14 9-10 9-13 11-14 12-13 27-29 27-33 28-34 28-38 29-30 30-31 31-32 32-33 34-35 35-36 36-37 37-38 exact/norm bonds : 3-20 7-16 10-17 12-19 13-18 17-28 18-27 29-40 30-39 36-41 exact bonds : 1-2 1-11 2-3 2-22 3-4 4-5 4-21 5-12 6-7 6-10 6-26 7-8 8-14 9-10 9-13  $9-24 \quad 11-14 \quad 11-25 \quad 12-13 \quad 12-23 \quad 27-29 \quad 27-33 \quad 28-34 \quad 28-38 \quad 29-30 \quad 30-31 \quad 31-32$ 31-44 32-33 34-35 35-36 35-42 35-45 36-37 37-38 37-46 39-43 isolated ring systems : containing 1 : 27 : 28 :

## Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS

## L3 STRUCTURE UPLOADED

=> s l3 ful FULL SEARCH INITIATED 09:03:09 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 1389 TO ITERATE

100.0% PROCESSED 1389 ITERATIONS SEARCH TIME: 00.00.01

0 ANSWERS

L4 0 SEA SSS FUL L3

=> => =>

Uploading C:\STNEXP4\QUERIES\10-648946b.str

```
chain nodes :
16 17 18 19 20 21 22 23 24 25 26 39 40 41 42 43 44 45 46 50
ring nodes :
1 2 3 4 5 6 7 8
                     9 10 11 12 13 14 27 28 29 30 31 32 33 34 35
36 37 38 47 48 49
chain bonds :
2-22 3-20 4-21 6-26 7-16 9-24 10-17
                                      11-25
                                            12-19 12-23 13-18 17-28 18-27
29-40 30-39 31-44 35-42 35-45 36-41
                                      37-46 39-43 48-50
ring bonds :
1-2 1-11 1-47 2-3 3-4 4-5 5-12 6-7 6-10 7-8 8-14 9-10 9-13 11-14
11-49 12-13 27-29 27-33 28-34 28-38 29-30 30-31 31-32 32-33 34-35 35-36 36-37 37-38 47-48 48-49
exact/norm bonds :
3-20 7-16 10-17 12-19 13-18 17-28 18-27 29-40 30-39 36-41 48-50
exact bonds :
1-2 1-11 1-47 2-3 2-22 3-4 4-5 4-21 5-12 6-7 6-10 6-26 7-8 8-14 9-10
9-13 9-24 11-14 11-25 11-49 12-13 12-23 27-29 27-33 28-34 28-38 29-30
30-31 31-32 31-44 32-33 34-35 35-36 35-42 35-45 36-37 37-38 37-46 39-43
47-48 48-49
isolated ring systems :
containing 1 : 27 : 28 :
```

## Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 49age 6s 42:CLASS 43:CLASS 44:CLASS 45:CLASS 47:Atom 48:Atom 49:Atom 50:CLASS

Page 7 10-648946

STRUCTURE UPLOADED L5

=> d

L5 HAS NO ANSWERS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s 15 ful

FULL SEARCH INITIATED 09:40:03 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED 29 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L5

=>

---Logging off of STN---

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 519.68 519.89

FULL ESTIMATED COST

STN INTERNATIONAL LOGOFF AT 09:52:03 ON 10 FEB 2005